Project 020 Development of NAS wide and Global Rapid Aviation Air Quality Tools

Massachusetts Institute of Technology (MIT)

Project Lead Investigator

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- P.I.: Steven R. H. Barrett
- FAA Award Number: 13-C-AJFE-MIT, Amendment Nos. 007, 018, 025, 032, and 041
- Period of Performance: Aug. 19, 2014 to Aug. 31, 2020
- Tasks:
  - Provide surface air quality analysis and quantify the impacts of aviation on surface air quality
  - Continue work on the development of nested domains and provide tool validation
  - Incorporate the nested domains into a single user-friendly framework
  - Support and assist the nvPM standard team on consistency-checking input data and interpreting results
  - Finalize and project uncertainty in ammonia emissions onto aviation impact sensitivities
  - Perform scoping of work for developing a multi-scale adjoint tool

Project Funding Level

$800,000 FAA funding + $50,000 Transport Canada funding = $850,000 total sponsored funds, with just $800,000 matching funds required. Sources of match are that same $50,000 Transport Canada funding (it constitutes both matching funds itself, as well as being sponsored funds that do not need to be matched), plus approximately $215,000 from MIT, and 3rd party in-kind contributions of $114,000 from Byogy Renewables, Inc. and $421,000 from Oliver Wyman Group.

Investigation Team (all MIT)

Principal Investigator: Prof. Steven Barrett
Co-Principal Investigator: Dr. Raymond L. Speth
Co-Investigator: Dr. Florian Allroggen
Research Scientist: Dr. Sebastian Eastham
Graduate students: Guillaume Chossière, Kingshuk Dasadhikari, Irene Dedoussi,

Project Overview

The aim of this project is to develop tools that enable the rapid assessment of the health impacts of aviation emissions. The focus of the project is on aviation-attributable $PM_{2.5}$ and ozone at the NAS-wide and global scales. These tools should allow for rapid policy analysis and scenario comparison. The adjoint method, which the tools are based on, provides a computationally efficient way of calculating the sensitivities of an objective function with respect to multiple model inputs. The project enhances the existing tools in terms of the domains and impacts covered, and in terms of uncertainty quantification. The enhanced tools support the FAA in its strategic vision to reduce the health impacts of aviation emissions, and allow for detailed and quantified policy analyses.

Tasks for Current and Next Period

Current Period (AY2017-2018)

- **Task 1:** Quantify surface air quality impacts of aviation
- **Task 2:** Continue work on the development of nested domains and provide tool validation
- **Task 3:** Operationalize the rapid assessment tool for internal use by the FAA
- **Task 4:** Support and assist the nvPM standard team (ASCENT 48) on consistency-checking input data and interpreting results
- **Task 5:** Finalize and project uncertainty in ammonia emissions onto aviation impact sensitivities
- **Take 6:** Perform scoping of work for developing a multi-scale adjoint tool

Next Period (AY2018-2020)

- **Task 1:** Extend the ASCENT 20 air quality assessment tool to account for high altitude aviation, including supersonic emissions
- **Task 2:** Quantify the impact of uncertainty in non-aviation emissions on calculated aviation emissions impacts
- **Task 3:** Extend operationalized MATLAB tools to account for the effect of non-aviation emissions uncertainty, and to include updated sensitivity matrices
- **Task 4:** Enable European regional simulations

Objectives

The aim of the project during this performance period is to enhance the capabilities of the existing rapid assessment tool. The main objectives of this cycle are aligned with the aforementioned tasks. Specifically:

1. Continue to work on the development of nested domains and provide tool validation. This will include code development and testing in order to develop a high-resolution simulation for Europe,
2. Operationalize tools and transition them to the FAA. The various model updates and the additions of the new nested domains with be packaged and wrapped with a user-friendly MATLAB script and will be passed to the FAA with a brief guidance document, similarly to the way the global and nested North American sensitivities were done,
3. Support and assist PM standard team in ensuring upstream input consistency (e.g. gridded emissions data) and results interpretation,
4. Quantify how uncertainties in the ammonia emissions propagate into the calculations of the adjoint sensitivities and how these affect the aviation attributable air quality impacts,
5. Perform scoping of work for developing a multi-scale adjoint tool that will enable the calculation of impacts from emissions occurring outside of the current nested domains, at the global scale. Perform comparison of aviation AQ impacts estimated using the global grid with the fine/nested grids' corresponding calculations.

Research Approach

As documented in previous reports, the central tool for this project is the GEOS-Chem adjoint. This reporting period has been dedicated to further extending the tool's capabilities as well as its validation. Significant work has also been invested in making the results of this project available for internal FAA use. This has allowed to us to produce and deliver to the FAA updated sensitivity maps for health impacts calculations and to provide insights into second-order sensitivity with respect to ammonia, which quantify the degree to which calculated aviation-impacts very with non-aviation ammonia emissions.

Quantification of the surface air quality impacts of aviation

In line with the main objectives of the ASCENT 20 project, our work for this period of performance has produced updated estimates of the impacts of national and global aviation on the surface air quality and has derived their associated health outcomes. The AEDT inventory for aviation year 2015 was used to produce these estimates, as well as the sensitivities derived from the GEOS-Chem adjoint. Below are some example results for calculating the health impacts surface air quality attributable to aviation NO_x emissions. Ozone impact calculations are a recent development for this project, and those calculated here are based on the Turner et al 2015 concentration response function (see Technical Guidance Document). This results in significantly greater mortality impacts than calculated previously using the older Jerrett et al 2010 concentration response function. Impacts due to $PM_{2.5}$ are also calculated using the Burnett et al 2014 integrated exposure response function, which finds lower impacts than the functions previously used for $PM_{2.5}$ impacts.

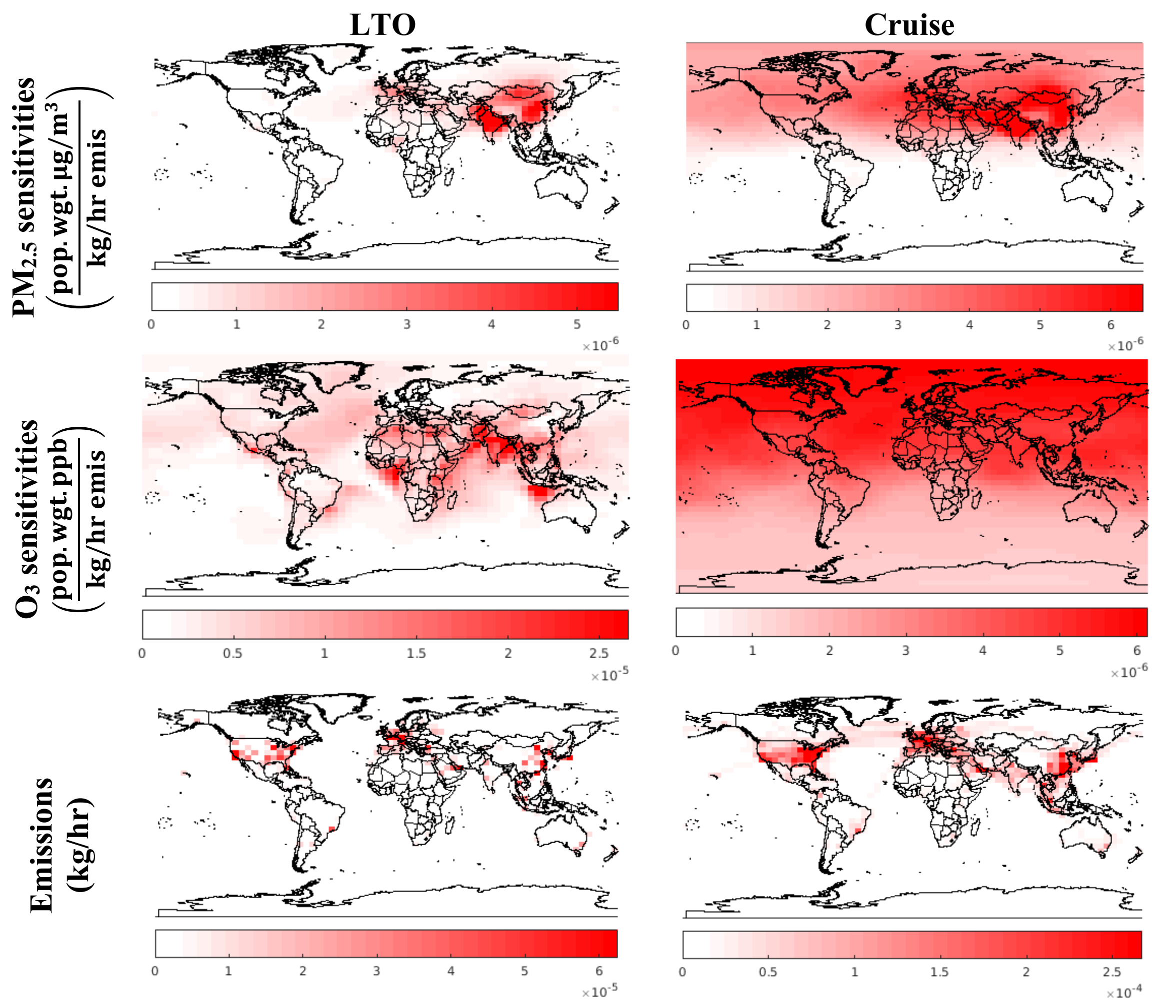

Figure 1. Global sensitivity to and aviation NO_x emissions in 2015. Color scales differ between panels to allow geographical distributions to be more easily resolved. Sensitivities show the annual average response.

Multiplying the emissions matrix for each species emitted by aviation element-wise by the corresponding sensitivity matrix and summing the products (the Technical Guidance document contains further details on these operations) allows us to compute the total health impacts of aviation 2015 emissions in each region. We find that uncertainties in the health-response function yields a 95% confidence interval of about (-49%, +50%).

Extension of the spatial capabilities of the tools and tool validation

Previous investigations using the North American nested domain have revealed that there are significant advantages to higher-resolution simulation over smaller domains. Capture of near-airport impacts is challenging with the coarse (~400 km) resolution at which the global model is run, while the finer (~50 km) resolution of the nested model is sufficient to isolate chemical and dynamical non-linearity associated with urban and coastal regions. This is complemented by further studies, such as Barrett et al (2010) and Eastham et al (2016), which show that the greatest impacts of aviation on surface air quality are incurred not in North America but rather in Western Europe and South Asia.

Accordingly, two additional nested domains were identified for use with the GEOS-Chem adjoint. The first is the South-East Asia nested domain. This domain, modeled at a resolution of 0.5˚×0.667˚, allows impacts of aviation to be finely resolved throughout India, China, Indonesia, and the rest of the South-East Asian domain. The domain is plotted in Figure 2. A similar grid is being developed and implemented for Europe.

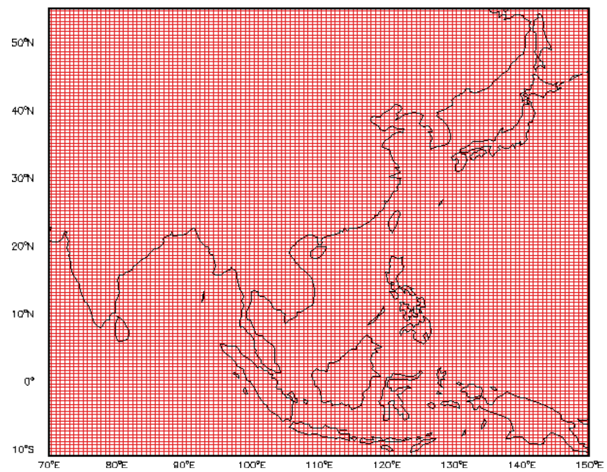

Figure 2. Fine-resolution domain covering Asia

Example sensitivity maps to aviation NO_x emissions for the nested Asia domain are shown in Figure 3. Beside committing work to capability extension, the project team has, during this past period of performance, conducted a validation of the tool by comparing the calculated health impacts attributable to aviation and due to exposure to $PM_{2.5}$ and ozone to the results obtained by modeling the impacts of aviation emissions on ground-level population exposure to $PM_{2.5}$ and ozone obtained from the forward model of GEOS-Chem. In both cases, the total health impacts were calculated using the gridded FAA AEDT-2015 aviation emissions. The comparisons between forward and adjoint results are presented in the Technical Guidance document delivered to the FAA along with the most up-to-date sensitivity data (see "Tool operationalization" section below). The error between the impacts computed using the forward and adjoint methods vary from 1% to 31%, with the highest error observed for the MDA-8 O_3 impacts for the Canadian receptor region. These errors are within the expected bounds for adjoint-based results.

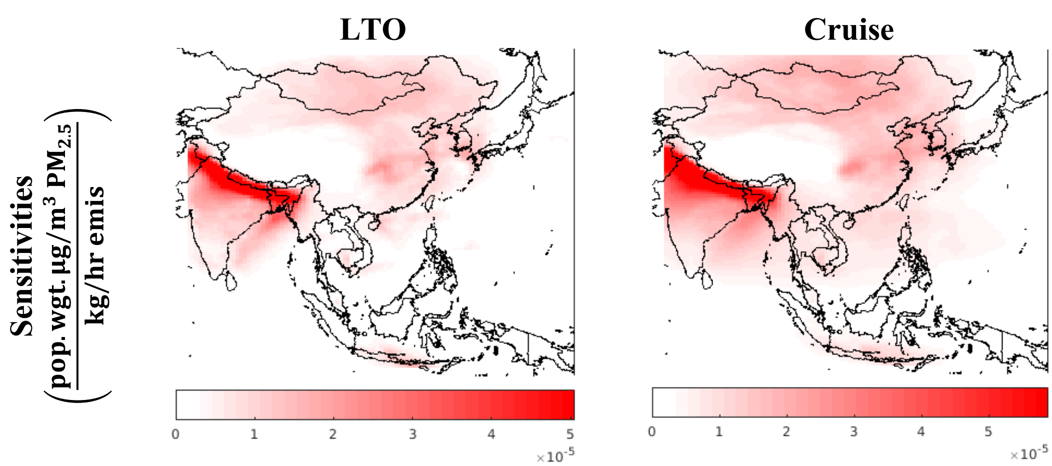

Figure 3. Example maps of the sensitivity of population-weighted $PM_{2.5}$ concentrations to aviation NO_x emissions during LTO (left) and at cruise altitude (right).

Tool operationalization

In this period of performance, the different model updates and the addition of the latest nested domains (namely Canada and Southeast Asia) have been packaged and wrapped in a MATLAB script to be delivered to the FAA along with the underlying data and supporting documentation on how the sensitivities were calculated and how to use them for practical health impacts calculations. This piece of software will be updated in the future as new domains become operational and as the air quality impacts assessment tool gets updated. Uncertainty analysis will also be included in this piece of software in the future. Please refer to the Technical Guidance document for further details on this part of this period of performance.

Support to PM standard (ASCENT Project 48)
This part of our objectives consisted mainly in assisting the PM standard team and ensuring data consistency in their inputs such as gridded emissions data. We also provided them with support in the interpretation of their results.

Ammonia uncertainty
Following a literature review and feasibility analysis, a key (and, as yet, unquantified) source of uncertainty is the potential impact of uncertainty in ammonia emissions on the sensitivity of air quality to aviation emissions. The rate of near-surface $PM_{2.5}$ formation is highly sensitive to local concentrations of ammonia, which acts to neutralize acidic aerosol and thereby increase the total aerosol mass. However, no study has yet incorporated the known high uncertainty in ammonia emissions into their estimates of health impacts from aviation.

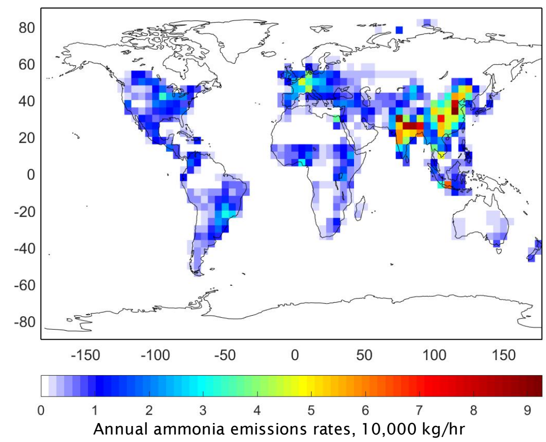

Figure 4. Baseline global ammonia emissions. Data are taken from the EDGAR v4.3.1 inventory.

A new strategy has been developed to estimate the impact of uncertainty in ammonia emissions on the sensitivity of average surface-level air quality to aviation emissions. This constitutes an application of the second-order sensitivity of aviation's impacts with respect to both aviation emissions and ammonia emissions, making use of the combined power of adjoint sensitivity calculation and forward differencing. We provide more details about this method and its application to project ASCENT 20 below. The global emissions that are currently used in the tool are plotted in Figure 4 at a resolution of 4°×5°. These emissions are taken from the EDGAR v4.3.1 inventory (Crippa et al. 2016), distributed as shown in Table 1.

Table 1. Baseline estimate of ammonia emissions by region

Region	Emission Total (Tg/Year)
Global	55.06 (*100%*)
China	14.02 (*25.5%*)
Other Asia	17.81 (*32.3%*)
Europe	5.65 (*10.3%*)
USA	4.17 (*7.57%*)
Other North America	2.11 (*3.83%*)
Other	11.24 (*20.4%*)

A key task performed during this period of performance was to estimate, from a literature review, the uncertainty associated with these regional ammonia inventories. The results are shown in Table 2. The column “Applied to” refers to the region to which the uncertainty was applied.

Table 2. Regionalized uncertainty in ammonia emissions

Region	Relative uncertainty	Applied to	Source
Global	(−18.75 %, +18.75 %)	Other	Beusen et al. (2008)
China	(−43 %, +50 %)	China, Other Asia	Zheng et al. (2012)
Europe	(−30 %, +30 %)	Europe	EMEP (2009)
USA	(−36 %, +36 %)	USA, Other NA	Zhu et al. (2012)

To compute the impact of these uncertainties in ammonia emissions on aviation-attributable health impacts, we first compute the first-order sensitivities of the desired health impacts to NH_3 emissions with and without aviation emissions. By multiplying the difference of these two matrices (whose values are expressed in units of $\frac{\mu g(PM_{2.5})/m^3}{kg(NH_3)/hr}$) by the uncertainty in ammonia emissions (in $\frac{kg\,(NH_3)}{hr}$), we compute, in each grid cell, the share of the uncertainty in the calculated total aviation-attributable impacts that can be traced back to uncertainties in ammonia emissions. The application of this method yielded the results shown in Table 3.

Table 3. Uncertainty in aviation impacts due to uncertainty in ammonia emissions

Summary	
Aviation-attributable, population-weighted $PM_{2.5}$	59.6 ng/m^3 (*baseline*)
NH_3-driven uncertainty	(−24.0, +27.0) ng/m^3 (*−40.2%, +45.5%*)
Regional Contributions to NH_3-Driven Uncertainty	**China:** (−11.9, +13.8) ng/m^3 (*−43.9%, +51.1%*) **Other Asia:** (−6.6, +7.7) ng/m^3 (*−24.5%, +28.5%*) **Europe:** ± 4.0 ng/m^3 (*± 6.7%*) **USA:** ± 1.1 ng/m^3 (*± 1.8%*) **Other NA:** ± 0.1 ng/m^3 (*± 0.4%*) **Other:** ± 0.2 ng/m^3 (*± 0.7%*)

Multi-scale adjoint tool

The development of a multiscale sensitivity analysis framework would combine the advantages of low-resolution global modeling for cruise sensitivity analysis with the advantages of high-resolution local modeling for resolving surface-level variations. Based on the work completed in this period of performance, a potential solution has been identified which would require to implement substantial modifications of the adjoint tool.

The proposed solution would involve re-engineering the adjoint to directly include sensitivity to changes in boundary conditions, supported by a finite-difference forward simulation to evaluate how the boundary conditions are affected by aviation. This effort would be supported by a multi-tier forward analysis to evaluate the difference in calculated impacts between the forward global, adjoint global, forward nested, and adjoint nested simulations.

Milestones

- *Surface air quality impacts of aviation*: Updated sensitivity to aviation emissions have been produced and used along with the AEDT 2015 inventory of aviation emissions to produce updated estimates of the health impacts of aviation emissions in different regions.
- *Nested domains and tool validation:* Work has continued on extending the capabilities of the tool to include high resolution modeling over various key regions. The tool was fully validated against the forward version of the GEOS-Chem model over all the operational domains.
- *Operationalize tools*: The various model updates and the additions of the new nested domains were packaged and wrapped into a user-friendly Matlab script that we passed to the FAA along with a brief guidance document.
- *Support PM standard analysis*: Support and assistance to the PM standard analysis team have continued, ensuring data consistency and providing help in result interpretation.
- *Ammonia uncertainty:* A full uncertainty quantification has estimated the share of the uncertainty in aviation-attributable health impacts that can be traced back to uncertainties in inventories of ammonia emissions.
- *Multi-scale adjoint modeling*: Scoping work was conducted for developing a multi-scale adjoint tool that will enable the calculation of impacts from emissions occurring outside of the current nested domains, at the global scale.

Major Accomplishments

During this period of performance, a validation of the tool in all of the operational geographical domain was performed. The tool was compared to calculations using the forward model of the global Chemical Transport Model GEOS-Chem. In addition, work has continued to enable higher resolution modeling over the European domain. Another key accomplishment during this period of performance was the quantification of the uncertainty in aviation-attributable health impacts that be linked to uncertainties in regional ammonia inventories. Finally, the tool was operationalized and packaged in a user-friendly MATLAB script, allowing the FAA to conduct air quality impacts analysis using up-to-date outputs from the air quality assessment tool.

Outreach Efforts

Results were presented at the 2018 ASCENT Spring and Fall meetings.

Student Involvement

Graduate students involved in this project are: Irene Dedoussi and Guillaume Chossière, PhD candidates in the Department of Aeronautics and Astronautics at MIT, and Kingshuk Dasidhakari, Masters student in the Department of Aeronautics and Astronautics at MIT.

Plans for Next Period

Over the next period of performance, we aim to improve our global impact assessment capabilities while quantifying key uncertainties in aviation's impacts on surface air quality. This includes novel applications of existing capabilities and the development of new capabilities, in order to both better characterize known uncertainties and to provide initial assessments of previously unquantified uncertainties. Data and model updated developed during the next period of performance will be packaged at the end of the year and passed to the FAA as updates to the MATLAB-based scripts provided during this period of performance. It will provide the FAA the ability to rapidly assess multiple aviation emissions scenarios in the context of uncertainties both internal and external to the aviation sector, as quantified by the work in this proposal. Following these overall objectives, we anticipate three major tasks to be undertaken by the ASCENT Project 20 team during the 2018/19 and 2019/2020 years.

Task 1 concerns the extension of the ASCENT 20 air quality assessment tool to account for high altitude aviation, including supersonic emissions. The adjoint model currently used for ASCENT project 20 to estimate sensitivity of population exposure to aviation was designed to capture the impacts of emissions within the troposphere and lower stratosphere. It is not yet capable of capturing impacts due to aviation at higher altitudes, particularly in the mid- or upper stratosphere, where supersonic aircraft would be expected to operate. The MIT Laboratory for Aviation and the Environment (LAE) has successfully extended the GEOS-Chem forward model, on which the adjoint is based, to simulate stratospheric chemistry and physics through the GEOS-Chem Unified Chemistry eXtension (UCX) (Eastham et al 2014). In order to accomplish this task, we will conduct a two-stage study to assess the impacts of projected supersonic aviation scenarios on surface air quality, including the differences in spatial pattern and in the timescale required to resolve the impacts. The first stage of the study will focus on single-case impact estimation using the validated forward model. The second stage of Task 1 will adapt and validate the adjointed version of the GEOS-Chem UCX model, which is currently under development at LAE for climate assessment purposes, to capture the sensitivity of air quality with respect to supersonic aviation.

Task 2 is an in-depth evaluation of the degree to which uncertainty in specific emissions related to non-aviation activities might affect the calculated impact of aviation. An initial estimate of the impact of uncertainty in ammonia emissions has revealed spatially heterogeneous relationships between ammonia emissions uncertainty and aviation emissions impacts. This pilot analysis has established a template for a broader assessment of these cross-sector second-order sensitivities, which are mathematically similar but functionally distinct from existing single-sector ("self") second-order sensitivities. In this task, we will use a combination of global and regional modeling to establish the degree of uncertainty which is propagated from background inventories of both anthropogenic ammonia, established during the previous project years as a key source of uncertainty in aviation's impacts, and in anthropogenic NO_x. This will require a thorough review of national- and regional-level uncertainties in emissions inventories for NO_x beyond the review for ammonia already underway.

For Task 3 we intend to package the sensitivity results from this year's and the previous years' efforts, to provide intuitive and consistent sensitivity matrices suitable for use in policy assessment. This includes not only the raw data but also MATLAB-based packages capable of accepting specific emissions scenarios and returning the expected air quality impacts. A central objective of this year's work would be to add multi-dimensional uncertainty quantification to the tool, including uncertainties in aviation emissions, uncertainty in background emissions of both ammonia and NO_x, and the impact functions themselves. This multi-dimensional assessment will be interpreted using a Monte Carlo analysis framework, which will provide the ability for any uncertainties already quantified through ASCENT project 20 to be propagated to the final impact estimate. Concurrent with this, we will provide an update to MIT's previous overview of the APMT-I Air Quality functionality in order to better reflect the latest air-quality-related functionalities. Ongoing work to enable European regional simulations, expected to be completed within the 2018-2020 period of performance, is included in this task.

References

Barrett, S. R. H., Britter, R. E., & Waitz, I. A. (2010). Global mortality attributable to aircraft cruise emissions. Environmental Science & Technology, 44(19), 7736–7742.

Beusen, A., Bouwman, A., Heuberger, P., Van Drecht, G., Van Der Hoek, K. (2008). Bottom-up uncertainty estimates of global ammonia emissions from global agricultural production systems. Atmos. Environ., 42 (2008), pp. 6067-6077

Eastham, S. D., D. K. Weisenstein, and S. R. H. Barrett (2014), Development and evaluation of the unified tropospheric-stratospheric chemistry extension (UCX) for the global chemistry-transport model GEOS-Chem, Atmos. Environ., 89, 52–63, doi:http://dx.doi.org/10.1016/j.atmosenv.2014.02.001

Eastham, S. D., & Barrett, S. R. H. (2016). Aviation-attributable ozone as a driver for changes in mortality related to air quality and skin cancer. Atmospheric Environment. https://doi.org/10.1016/j.atmosenv.2016.08.040

European Commission Joint Research Centre (JRC) and Netherlands Environmental Assessment Agency (PBL). (2014). Emission Database for Global Atmospheric Research (EDGAR), release EDGARv4.2 FT2012 [Data set]. Retrieved from http://edgar.jrc.ec.europa.eu

European Monitoring and Evaluation Program Centre on Emission Inventories and Projections (EMEP). WebDab Emissions Database. http://www.ceip.at/ms/ceip_home1/ceip_home/webdab_emepdatabase/reported_emissiondata/

Zhang, Q., Streets, D. G., Carmichael, G. R., He, K. B., Huo, H., Kannari, A., … Yao, Z. L. (2009). Asian emissions in 2006 for the NASA INTEX-B mission. Atmospheric Chemistry and Physics, 9(14), 5131–5153.

Zheng, J.Y., Yin, S.S., Kang, D.W., Che, W.W., Zhong, L.J. (2012). Development and uncertainty analysis of a high-resolution NH_3 emissions inventory and its implications with precipitation over the Pearl River Delta region, China. Atmos. Chem. Phys., 12 pp. 7041-7058

Zhu, L., D. K. Henze, K. E. Cady-Pereira, M. W. Shephard, M. Luo, R. W. Pinder, J. O. Bash, and G.-R. Jeong (2013), Constraining U.S. ammonia emissions using TES remote sensing observations and the GEOS-Chem adjoint model, J. Geophys. Res. Atmos., 118, 3355–3368, doi: 10.1002/jgrd.50166.